

Simple Construction of High Order Rational Iterative Equation Solvers

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Simple Construction of High Order Rational Iterative Equation Solvers

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Abstract

This article proposes a general technique to construct arbitrarily high order rational *one-point* iterative equation solvers based on truncated Taylor expansion from lower order schemes. With adding one more function call, an iterative equation solver of convergence order n can be accelerated to order (2n-1). Many existing (some recently published) one-point and two-point iterative equation solvers are special cases of the proposed construction. The proposed approach may be used to obtain new iterative equation solvers.

TAYLOR EXPANSION AND THE ORDER OF CONVERGENCE OF AN ITERATIVE SOLVER

An one-point iterative equation solver for f(x) = 0 can be generally written as a fixed-point iteration as

$$x_{k+1} = x_k + \delta(f(x_k), f'(x_k), f''(x_k)...) = x_k + \delta_k.$$
(1)

If the solver is of convergence order n, we also have

$$f(x_k + \delta_k) = O(\delta_k^n). (2)$$

With a finite Taylor expansion of the equation above we have

$$f(x_k + \delta_k) \sim f + f'\delta_k + \frac{f''}{2}\delta_k^2 + \dots + \frac{f^{(n-1)}}{(n-1)!}\delta_k^{n-1} = O(\delta_k^n).$$
 (3)

Take n=2 and ignore terms that has same of higher orders, one has $f(x_k+\delta_k) \sim f + f'\delta_k = 0$. Solve for δ_k one arrives at the well-known Newton's method^[4]

$$\delta_k = -\frac{f(x_k)}{f'(x_k)},\tag{4}$$

and the expression of δ_k is rational function of f, f'.

Take n=3 and ignore terms that have same of higher orders, one has $f(x_k + \delta_k) \sim f + f' \delta_k + f'' \delta_k^2 / 2 = 0$. Solve for δ_k one arrives at the famous Halley's irrational method^[5]

$$\delta_k = \frac{\operatorname{sgn}(f'(x_k))}{f''(x_k)} \left(\sqrt{(f'(x_k))^2 - 2f(x_k)f''(x_k)} - |f'(x_k)| \right), \tag{5}$$

but the expression is already irrational.

For n = 4, 5, explicit, irrational solutions of truncated Taylor expansions are available but difficult to implement; for n > 5 no general explicit solution is available^[3].

In all the derivations later we assume the first derivative of f(x) is non-zero at the solution.

RATIONAL HIGH-ORDER EQUATION SOLVERS

To avoid irrational expressions of an iterative equation solver, we may use *lower-order* rational iterative solvers to construct higher order solvers. For example, for n = 3, we write the equation for truncated Taylor expansion as (dropping the subscript k for simplicity)

$$f + \delta(f' + \frac{f''}{2}\delta) = 0.$$

We then use the Newton's second-order solution $\delta_{newton} = -f/f'$ to substitute the δ inside the parenthesis and obtain

$$f + \delta(f' - \frac{f''}{2}\delta_{newton}) \sim f + \delta(f' - \frac{ff''}{2f'}) = 0.$$

Solve for δ we obtain Halley's rational method that

$$\delta_{halley} = -\frac{2ff''}{2(f')^2 - ff''},\tag{6}$$

which is a rational method.

In general if some lower order methods have been constructed that obtain and we have for each i = 2, 3,(n-1) a rational method that is i^{th} -order convergent till i = n - 1. A n^{th} -order can be constructed with

$$f + \delta(f' + \frac{f''}{2}\Delta + \dots + \frac{f^{(n-1)}}{(n-1)!}\Delta^{n-2}) = 0,$$
(7)

where Δ is a $(n-1)^{th}$ -order solution. Then one obtains

$$\delta = -\frac{f}{f' + \frac{f''}{2}\Delta + \dots + \frac{f^{(n-1)}}{(n-1)!}\Delta^{n-2}}.$$

Now we prove the above construction gives an iterative method of order n. The above equation can be written as

$$f(x) + \delta(f' + \frac{f''}{2}\Delta + \dots + \frac{f^{(n-1)}}{(n-1)!}\Delta^{n-2}) = 0.$$
 (8)

Because Δ is a $(n-1)^{th}$ -order solution we have, $f(x+\Delta)=O(\Delta^{n-1})$ and the Taylor expansion

$$f(x + \Delta_{n-1}) = f(x) + \Delta(f' + \frac{f''}{2}\Delta + \dots + \frac{f^{(n-2)}}{(n-2)!}\Delta^{n-3}) = O(\Delta^{n-1}).$$
 (9)

Subtracting eq. (9) form eq. (8) one has

$$(\delta - \Delta)(f' + \frac{f''}{2}\Delta + \dots + \frac{f^{(n-2)}}{(n-2)!}\Delta^{n-3}) = O(\Delta^{n-1}, \delta\Delta^{n-2}).$$
 (10)

This tell us that δ and Δ are of the same order for n > 2 and

$$(\delta - \Delta) = O(\Delta^{n-1}).$$

We expand $f(x + \delta^{[n]})$ to order n and observe that

$$f(x+\delta) = f + f'\delta + \frac{f''}{2}\delta^2 + \dots + \frac{f^{(n-1)}}{(n-1)!}\delta^{n-1} + O(\delta^n).$$
 (11)

Subtracting eq. (8) from the above equation one finds that

$$f(x+\delta) = \delta(\frac{f''}{2}\Delta(\delta-\Delta) + \dots + \frac{f^{(n-1)}}{(n-1)!}(\delta^{n-1} - \Delta^{n-1})) + O(\delta^n).$$
 (12)

However with applying the result that $\delta - \Delta = O(\Delta^{n-1})$ from eq. (10)we have

$$f(x+\delta) = O(\delta^n). (13)$$

Thus eq. (7) is a n^{th} -order convergent equation solving scheme and it is a rational one.

SIMPLIFIED HIGH-ORDER ITERATIONS

Because a higher order scheme is in general more complex than a lower order scheme, it is desired to reduce the complexity of the n^{th} -order scheme with schemes of orders lower than (n-1) to replace the $(n-1)^{th}$ -order scheme as much as possible. A possibility is to solve

$$f + \hat{\delta}(f' + \frac{f''}{2}\Delta_{[n-1]} + \frac{f'''}{6}\Delta_{[n-2]}\dots + \frac{f^{(n-1)}}{(n-1)!}\Delta_{[2]}^{n-2}) = 0,$$
 (14)

where $\Delta_{[i]}$ is solution of an i^{th} -order scheme, and solve for $\hat{\delta}$.

The pattern here is that each m^{th} derivative $f^{(m)}$ with m > 2, has a multiplier of at least a $(n+1-m)^{th}$ -order iterative solution. Taking a solution with a higher order in any of the terms would always works but does not increase the overall order of convergence. Since a lower order Δ is simpler in expression than a higher order Δ , eq. (14) provides a simpler scheme than eq. (7), however the solution is also n^{th} -order and it can be proven as described below.

We are about the evaluate the difference between δ in eq. (7) and $\hat{\delta}$ in eq. (14). We have

$$\hat{\delta} - \delta = f(x)(T_1^{-1} - T_2^{-1}) = \frac{f(x)}{T_1 T_2}(T_2 - T_1),$$

where the terms T_1 and T_2 are defined as

$$T_1 = f' + \frac{f''}{2} \Delta_{[n-1]} + \frac{f'''}{6} \Delta_{[n-2]} \dots + \frac{f^{(n-1)}}{(n-1)!} \Delta_{[2]}^{n-2},$$

and

$$T_2 = f' + \frac{f''}{2} \Delta_{[n-1]} + \frac{f'''}{6} \Delta_{[n-1]} \dots + \frac{f^{(n-1)}}{(n-1)!} \Delta_{[n-1]}^{n-2}.$$

Therefore

$$T_2 - T_1 = \frac{f'''}{6} (\Delta_{[n-1]}^2 - \Delta_{[n-2]}^2) + \dots + \frac{f^{(n-1)}}{(n-1)!} (\Delta_{[n-1]}^{n-2} - \Delta_{[2]}^{n-2}).$$
 (15)

Next we evaluate the sizes of the term $(\Delta_{[n-1]}^m - \Delta_{[n-m]}^m)$ for m=2,3,...,n-2. By definition one has the following

$$f(x + \Delta_{[n-1]}) = O(\Delta_{[n-1]}^{n-1}),$$

and

$$f(x + \Delta_{[n-m]}) = O(\Delta_{[n-m]}^{n-m}).$$

Take the difference between the two expressions one finds that

$$f(x + \Delta_{[n-1]}) - f(x + \Delta_{[n-m]}) = f'(\theta)(\Delta_{[n-1]} - \Delta_{[n-m]}) = O(\Delta_{[n-m]}^{n-m}), \tag{16}$$

where θ is some point between $x + \Delta_{[n-1]}$ and $x + \Delta_{[n-m]}$, by the mean-value theorem.

Therefore we have $\Delta_{[n-1]}$ and $\Delta_{[n-m]}$ are of the same order Δ , and then use eq. (16), we arrive at

$$(\Delta_{[n-1]}^m - \Delta_{[n-m]}^m) = (\Delta_{[n-1]} - \Delta_{[n-m]})O(\Delta^{m-1}) = O(\Delta^{n-1}).$$
 (17)

Because the above is true, this time eq. (15) becomes

$$T_2 - T_1 = \frac{f'''}{6} (\Delta_{[n-1]}^2 - \Delta_{[n-2]}^2) + \dots + \frac{f^{(n-1)}}{(n-1)!} (\Delta_{[n-1]}^{n-2} - \Delta_{[2]}^{n-2}) = O(\Delta^{n-1}).$$

Thus

$$\hat{\delta} - \delta = \frac{f(x)}{T_1 T_2} (T_2 - T_1) = f(x) O(\Delta^{n-1}).$$

However $f(x) = O(\Delta)$ because $f(x + \Delta) = f(x) + f'(x)\Delta + ... = o(\Delta)$ by definition of order of convergence for each $\Delta_{[i]}$ involved in our discussion, therefore we have

$$\hat{\delta} - \delta = O(\Delta^n),\tag{18}$$

which means

$$\hat{\delta} = -\frac{f(x)}{f' + \frac{f''}{2}\Delta_{[n-1]} + \frac{f'''}{6}\Delta_{[n-2]}^2 \dots + \frac{f^{(n-1)}}{(n-1)!}\Delta_{[2]}^{n-2}}$$

provides a n^{th} -order convergent iterative equation solver

$$x_{k+1} = x_k + \hat{\delta}(x_k). \tag{19}$$

ACCELERATED ITERATIVE EQUATION SOLVERS

For a one-point iteration scheme of a convergence order n with

$$x_{k+1} = x_k + \hat{\delta}(x_k)$$

where $\hat{\delta}(x_k) = \hat{\delta}(f(x_k), f'(x_k), ..., f^{(n-1)}(x_k))$, adding one function call $f(x_{k+1})$ to $f(x_k)$ will raise the order of convergence from n to (2n-1). This is to say that the scheme follows

$$\hat{x}_{k+1} = x_k + \hat{\delta}(f(x_k) + f(x_{k+1}), f'(x_k), ..., f^{(n-1)}(x_k)), \tag{20}$$

is $(2n-1)^{th}$ -order convergent^[3]. Since we are now able to construct an *one-point* iterative solver with an arbitrary order of convergence with eq. (19), it is desired to accelerate it to order (2n-1) by adding just one function call.

Next we list some accelerated iterative schemes constructed by the approach described in the last section.

ACCELERATED THIRD ORDER NEWTON SCHEME

The Newton's method eq. (4) is accelerated to a third-order scheme

$$x_{k+1} = x_k - \frac{f(x_k) + f(y_k)}{f'(x_k)},$$
(21)

where $y_k = x_k - f(x_k)/f'(x_k)$. Three function calls are needed for the *third-order*, its efficiency-index^[2] is $\sqrt[3]{3} = 1.442$. The accelerated scheme^[8] is faster than Newton's original method with an efficiency-index $\sqrt{2} = 1.414$.

ACCELERATED FIFTH ORDER HALLEY SCHEMES

The Halley's irrational scheme eq .(5) can be accelerated to fifth-order^[6] by solving again that

$$f(x_k) + f(x_k + \delta_k) + f'(x_k)\Delta_k + \frac{f''(x_k)}{2}\Delta_k^2 = 0,$$

with

$$x_{k+1} = x_k + \Delta_k. (22)$$

However with our construction method eq. (19) for n = 3, we have the third-order rational Halley's method eq. (6), and it can be accelerated to a fifth-order scheme^[7] by adding one function calls that

$$y_k = x_k - \frac{2f(x_k)f(x_k)''}{2(f(x_k)')^2 - f(x_k)f''(x_k)},$$

$$x_{k+1} = x_k - \frac{2(f(x_k) + f(y_k))f(x_k)''}{2(f(x_k)')^2 - (f(x_k) + f(y_k))f''(x_k)}.$$
(23)

ACCELERATED SEVENTH ORDER SCHEMES

With our construction method eq. (19) for n = 4, a rational seventh-order scheme can be constructed as

$$\hat{\delta}_{4th} = -\frac{f}{f' + \frac{f''}{2} \Delta_{Halley} + \frac{f'''}{6} \Delta_{Newton}^2},$$

where Δ_{Halley} is defines by eq. (6) and Δ_{Newton} is the original Newton's solution by eq. (4). This fourth-order scheme can be accelerated to seventh-order and the solution can be written as

$$y_k = x_k + \hat{\delta}_{4th},$$

$$x_{k+1} = x_k - \frac{f(x_k) + f(y_k)}{f'(x_k) - \frac{(f(x_k) + f(y_k))(f''(x_k))^2}{2(f')^2 - (f(x_k) + f(y_k))f''} + \frac{f(x_k)'''(f(x_k) + f(y_k))^2}{6(f'(x_k))^2}}.$$
(24)

In the above construction, Δ_{Newton} can be replaced by any rational iterative solution that is second-order or higher (say, Δ_{Halley}) and one obtains a different seventh-order scheme. Δ_{Halley} can be any other third-order, one-point iterative solution. For example, with Halley's irrational solution to construct $\hat{\delta}_{4th}$, then by adding $f(y_k)$ to $f(x_k)$ and reapply the fourth-order iteration, one obtains another seventh-order method. However this time the scheme is irrational.

HIGHER-ORDER ITERATIVE SCHEMES

In principle, given an arbitrarily specified convergence order n, an rational iterative equation solver of convergence order n can always be constructed. For simplicity lower-order schemes should be employed whenever possible and we believe eq. 19) gives the least complicated construction of this type of rational iterative solvers.

However, by mixing and matching *lower-order* schemes, there is a combination explosion of the way to construct n^{th} -order one-point iterative solvers by the approach described in this paper.

With adding a single function call $f(x+\hat{\delta})$ to f(x) replacing f(x) in a *one-point* iterative equation solver, its order of convergence is raised to 2n-1.

CONCLUSION

By consecutively applying lower-order rational iterative solutions with a truncated Taylor expansion of $f(x+\delta)$ to order n and obtain a linear equation of δ , an iterative solver of arbitrary n^{th} -order convergence can be constructed. By adding $f(x+\delta)$ to f(x) in the n^{th} -order scheme obtained and reapply the scheme, a $(2n-1)^{th}$ -order convergent iterative scheme can be constructed. Many existing iterative solvers are just special cases of this construction. It is possible to construct new high-order iterative equation solvers with this construction.

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REFERENCE

- [1]. H. T. Kung and J. F. Traub "Optimal Order of One-Point and Multi-Point Iteration", *Journal of the Association for Computing Machinery*, Vol. 21, No. 4, pp.643-651, 1974.
- [2]. A. M. Ostrowski, "Solution of Equations and System of Equations", *Pure and Applied Mathematics*, vol. 9, Academic Press, New York, (1966).
- [3]. J. Yao, "An Easy Method To Accelerate an Iterative Algebraic Equation Solver", Journal of Computational Physics, to appear.
- [4]. Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P., *Numerical Recipes in C*, second edition, Cambridge University Press, (1997).

- [5]. Weisstein, E. W. "Halley's Irrational Method", From *MathWorld* A Wolfram Web Resource.
- [6]. M. Grau and M. Nogurea, "A Variant of Cauchy's Method with Accelerated Fifth-Order Convergence", *Applied Mathematics Letters* 17, pp.509-517, (2004).
- [7]. M. A. Noor, W. A. Khan, and A. Hussain, "A new modified Halley method without second derivatives for nonlinear equation", *Applied Mathematics and Computation* 189, pp.1268-1273, 2007.
- [8]. C. Chun, "A simply constructed third-order modifications of Newton's method", *Journal of Computational and Applied Mathematics*, Vol. 215, Issue 1, pp.81-89, 2008.